

Quantum and Dirac Materials for Energy Applications Conference



La Fonda on the Plaza - Santa Fe
March 8 to 11, 2015

Welcome to the *Quantum and Dirac Materials for Energy Applications Conference (QDM-15)*. This conference follows the *Competing Orders in Functional Materials and their Applications Workshop*, which was held at Nordita in Stockholm, Sweden in June of 2013.

The *Quantum and Dirac Materials for Energy Applications Conference* is hosted by the Institute for Materials Science (IMS) at Los Alamos National Laboratory, the Royal Institute of Technology (KTH), Nordita and the New Mexico Consortium (NMC) at La Fonda on the Plaza in Santa Fe, New Mexico from March 8 to March 11.

QDM-15 will highlight recent developments in the synthesis and characterization of novel materials like Dirac materials and emphasize the importance of combined theory and modeling together with the advanced spectroscopies of materials.

The purpose of the workshop is to discuss current status and future prospects for the quantum materials and Dirac materials for energy and information technology applications using recent advances in synthesis, characterization and modeling. We will pay particular attention to the nonequilibrium and pumped probes of materials and Dirac materials.

We are pleased to host a broad scope of speakers that will cover these topics in an informal setting allowing significant time for informal discussions.

An essential part of the IMS mission is to engage in and develop long-term collaborations between United States and international institutions. IMS has put forth a memorandum of understanding between KTH/Nordita and Los Alamos National Laboratory. This Memorandum Of Understanding has now been signed and this conference will mark a new step in development of these collaborations

Following the scientific portion of the conference on March 8th, 9th and the morning of the 10th, there will be several presentations and round tables. We will make use of the round tables to discuss future initiatives and collaborative efforts between the hosts of this conference, the Royal Institute of Technology, Nordita and Institute for Materials Science at Los Alamos National Laboratory.



Quantum and Dirac Materials for Energy Applications Conference

March 8-11, 2015

Organizing Committee:

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Session Chairs:

Sunday afternoon: Alexander Balatsky

Monday morning: Avadh Saxena

Monday afternoon: David Abergel

Tuesday afternoon: Ulf Karlsson

Speakers:

Daved Abregel

Alexander (Sasha) Balatsky

Christian Batista

Alan Bishop

Dave Clark

John Davis

Jonathan Edge

Olaf Eriksson

Waclaw Gudowski

Philip Hofmann

Leif Kari

Ulf Karlsson

Martin Månsson

Ross McDonald

Aditya Mohite

Jens Paaske

Filip Ronning

Enrico Rossi

John Sarrao

Avadh Saxena

Thorsten Schmitt

Edbert J. Sie

Antoinette (Toni) Taylor

Oscar Tjernberg

Dmitry Yarotski

Jian-Xin Zhu

Wojciech Zurek

Roundtables:

Moderators

Round Table 1

Avadh Saxena and Ulf Karlsson

Round Table 2

Nate Mara and
Waclaw Gudowski

Round Table 3

Jeff Wills, Alexander Balatsky
and Olaf Eriksson

Participants

C. Mielke, A. Taylor, Q. Jia, J. Sarrao,
C. Barnes, A. Bishop (LANL); U. Karlsson,
M. Månsson, (KTH); J. Fransson (UU)

M. Caro, O. Anderoglu, N. Mara (LANL);
W. Gudowski (KTH)

J. Wills, J. Zhu, C. Batista, J. Sarrao, A. Taylor,
A. Bishop, D. Clark (LANL); O. Eriksson (UU)



QDM-15 Conference - Timetable Summary

Sunday, March 8th 2015

11:00 - 13:00	Arrival and Registration
13:00 – 17:00	Kick-off Afternoon Session in the <u>New Mexico Meeting Room</u>
13:00—13:10	D. Clark: <i>Welcome</i>
13:10 – 13:20	A. Balatsky: <i>Organization and General Comments</i>
13:20—14:00	A. Saxena: <i>Mesoscale and Multiferroics</i>
14:00—14:40	O. Eriksson: <i>Multipurpose Electronic Database for Correlated Systems</i>
14:40—15:20	C. Batista: <i>Skyrmions and Frustration</i>
15:20—15:40	Break
15:40—14:20	E. Rossi: <i>Kondo Effect and Non Fermi Liquid Behavior in Dirac Materials</i>
16:20—17:00	F. Ronning: <i>The "115" Superconductors</i>
17:00—17:40	W. Zurek: <i>Quench in Quantum Phase Transitions</i>
18:00—19:00	QDM Meeting Reception at <u>La Fonda Terraza</u>
19:00—23:00	QDM Banquet Dinner at <u>La Fonda Terraza</u> (reservation required)

Monday, March 9th 2015

7:30—9:00	Breakfast in the <u>Santa Fe Meeting Room</u> (provided by La Fonda Hotel)
9:00—12:00	Morning session in the <u>New Mexico Meeting Room</u>
9:00—9:40	JC Séamus Davis: <i>Atomic-scale Imaging of Dirac-Mass Configurations in Ferromagnetic Topological Insulators</i>
9:40—10:20	J.X. Zhu: <i>Local Electronic Structure and Inhomogeneity in Heavy Fermion System</i>
10:20—10:40	Break
10:40—11:20	P. Hofmann: <i>Electronic Structure and Electron Dynamics in Two-Dimensional Materials</i>
11:20—Noon	A. Balatsky: <i>Dirac Materials</i>
Noon—13:20	Break for Lunch at <u>La Terraza</u> (provided by La Fonda Hotel)
13:20—17:00	Afternoon Session in the <u>New Mexico Meeting Room</u>
13:20—14:00	R. McDonald: <i>Topological Surface States in the Quantum Limit</i>
14:00—14:40	D. Yarotski: <i>Pumped Probes and Topological States</i>
14:40—15:00	Break
15:00—15:40	A. Mohite: <i>Properties of Chalcogenites</i>
15:40—16:00	M. Månsson: <i>Towards Sodium-based Solid State Energy Storage</i>
16:00—16:40	O. Tjernberg: <i>ARPES on Crystalline Topological Insulators</i>
17:00—19:30	Speaker – Participant discussions



QDM-15 Conference - Timetable Summary (continued)

Tuesday, March 10th 2015

7:30—9:00	Breakfast in the <u>Santa Fe Meeting Room</u> (provided by La Fonda Hotel)
9:00—12:00	Morning session in the <u>New Mexico Meeting Room</u>
9:00—9:40	J. Edge: <i>Multiband Effects in Interfacial Superconductors</i>
9:40—10:00	J. Paaske: <i>Yu-Shiba-Rusinov States and Edge Zero Modes in Superconductors</i>
10:00—10:20	Break
10:20—11:00	D. Abregel: <i>One Dimensional Excitons</i>
11:00—11:30	T. Schmitt: <i>Resonant Inelastic X-Ray Scattering on One-Dimensional Cuprate and Oxide Heterostructure Materials</i>
11:30—12:00	E.J. Sie (Gedik Group): <i>Breaking Time-reversal Symmetry in WS₂ with Light</i>
12:00—12:40	A. Taylor: <i>Ultrafast Dynamics in Correlated Electron Materials</i>
12:40—13:30	Break for Lunch at <u>La Terraza</u> (provided by La Fonda Hotel)
13:30—17:40	Afternoon Session in the <u>New Mexico Meeting Room</u>
13:30—13:45	L. Kari- Dean, School of Science: <i>Research at KTH</i>
13:45—14:00	A. Bishop - Principle Associate Lab Director: <i>Research at Los Alamos</i>
14:00—14:15	U. Karlsson – Professor and Materials Platform Head: <i>KTH Materials Platform</i>
14:15—14:30	J. Sarrao - Associate Lab Director: <i>Theory, Experiment Matter in Extreme Conditions</i>
14:30—14:45	W. Gudowski , PI, Head: <i>Nuclear Reactor Research in KTH</i>
Round table 1	Materials for Nuclear Energy - Nuclear reactor safety and Nuclear Energy Programs
Round table 2	Computational Materials Initiative And F- Electron Actinide Materials Database
Round table 3	Materials In Extreme - Magnet Lab, MARIE, LUMOS, CINT
17:00—19:30	Summary of Round table discussions and discussion wrap-up

Wednesday, March 11th 2015

7:30—9:00	Breakfast in the <u>Stiha Room</u> (provided by La Fonda Hotel)
9:00—12:00	Morning session in the <u>Stiha Room</u> (with short coffee break)
9:00—Noon	Round Table wind-up session (<i>end time is tentative</i>)
12:45	Meet in front of Hotel Reception for transportation to Los Alamos
12:55 – 14:00	Travel to Los Alamos National Laboratory
14:00 – 14:30	Los Alamos Badge office to get badges
14:30—17:45	Tour of Los Alamos Facility – by pre-arrangement with A. Balatsky
14:30 – 15:30	CINT tour - Jia Quanxi
15:30 – 16:00	CNLS tour - Robert Ecke and Aric Hagberg
16:15 – 17:45	NHMFL tour - Charles Mielke



Quantum and Dirac Materials for Energy Applications Conference - Detailed Timetable

Sunday, March 8th 2015

- 11:00 - 13:00 **Arrival and Registration**
Hotel Check-in at La Fonda on the Plaza – Santa Fe, New Mexico
Conference Registration and material pick-up at the Portal
- 13:00 – 17:00 Kick-off Afternoon Session in the New Mexico Meeting Room
- 13:00—13:10 **D. Clark:** *Welcome*
- 13:10 – 13:20 **A. Balatsky:** *Organization and General Comments*
- 13:20—14:00 **A. Saxena:** *Mesoscale and Multiferroics*
- 14:00—14:40 **O. Eriksson:** *Multipurpose Electronic Database for Correlated Systems*
- 14:40—15:20 **C. Batista:** *Skyrmions and Frustration*
- 15:20—15:40 **Break**

- 15:40—14:20 **E. Rossi:** *Kondo Effect and Non Fermi Liquid Behavior in Dirac Materials*
- We study the Kondo effect in three-dimensional (3D) and two-dimensional (2D) Dirac materials [1]. We find the scaling of the Kondo temperature with respect to the doping n and the coupling J between the moment of the magnetic impurity and the carriers of the semimetal, we obtain the scaling with respect to the doping of the resistivity due to the Kondo effect. We also study the effect of the interplay of long-range scalar disorder and Kondo effect. In the presence of disorder-induced, long-range, carrier density inhomogeneities the Kondo effect is not characterized by a Kondo temperature but by a distribution of Kondo temperatures. We obtain the expression of such distribution and show that its features cause the appearance of strong non-Fermi liquid behavior. [1] A. Principi, G. Vignale, E. Rossi, arXiv:1410.8532.
- 16:20—17:00 **F. Ronning:** *The "115" Superconductors*
- The compounds CeMIn_5 ($M=\text{Co, Rh, Ir}$) are known as the "115" superconductors. Because of their high purity and the small energy scales present in these heavy fermion materials, they are ideal model systems through which to explore the interplay between magnetism and superconductivity, which are present in many classes of unconventional superconductors. After a brief introduction into the 115s, I will review some of our recent results. In particular, NMR investigations of Cd versus Sn dopants on the In sites, which reveal different degrees of electronic heterogeneity. Importantly, the degree of inhomogeneity strongly influences the non-Fermi liquid signatures at the quantum critical point as well as the suppression of superconductivity. Additionally, transport studies on micro patterned crystals of CeRhIn_5 under high magnetic fields reveals a density wave state akin to what has been observed in cuprates, accompanied by a strong dimensional reduction.
- 17:00—17:40 **W. Zurek:** *Quench in Quantum Phase Transitions*
- 18:00—19:00 **QDM Meeting Reception at La Fonda Terraza**
- 19:00—23:00 **QDM Banquet Dinner at La Fonda Terraza (reservation required)**



Monday, March 9th 2015

7:30—9:00 **Breakfast** in the Santa Fe Meeting Room (provided by La Fonda Hotel)

9:00—12:00 Morning session in the New Mexico Meeting Room

9:00—9:40 **JC Séamus Davis:** *Atomic-scale Imaging of Dirac-Mass Configurations in Ferromagnetic Topological Insulators*

The existence of the Dirac surface states of topological insulators (TI) is now well established. Novel physics can be achieved using these states, if an energy gap can be opened in their Dirac-like spectrum. This should generate many highly exotic new properties including the quantum anomalous Hall effect (QAHE), axionic electrodynamics, and even electric-field induced magnetic monopoles. However, after almost a decade of research into TI materials, these phenomena have proven extremely elusive. To explore this mystery, we recently introduced the Dirac-mass 'gapmap' technique to visualize the atomic-scale spatial conformations of Dirac mass [1]. It reveals new perspectives on the physics of ferromagnetic topological insulators. By simultaneously visualizing the mass gap $\Delta(r)$ and the ferromagnetic dopant atoms, we discover intense nanoscale disorder in the Dirac-mass and demonstrate that this is directly related to fluctuations in the magnetic-dopant atom density $n(r)$. The key realization from these data is that, in TIs controlled by magnetic-dopant atom phenomena, the primary chiral edge states at the sample boundary can hybridize through the percolating internal edges at the $\Delta(r)$ domain walls so that the QAHE (and likely all other gapped-TI surface state phenomena) will be heavily suppressed. Therefore, to reliably achieve the exotic physics expected of time-reversal symmetry breaking TI materials, it now appears that understanding and control of dopant-induced Dirac-mass gap disorder will first need to be achieved.

9:40—10:20 **J.X. Zhu:** *Local Electronic Structure and Inhomogeneity in Heavy Fermion System*

The intermetallic heavy fermion compounds based on either rare earth elements or on actinides are prototypical strongly correlated systems. In these materials, the interplay between the hybridization of local f -electrons with conduction electrons and the screened on-site Coulomb repulsion gives rise to wide range of behaviors, including magnetic ordering, Fermi liquid and non-Fermi liquid.

In this talk, I will discuss the electronic inhomogeneity and local electronic structure around impurities in these systems. I first show that, for certain carrier concentrations, the uniform Fermi liquid becomes unstable with respect to formation of a new kind of anharmonic "Kondo stripe" state with inhomogeneous Kondo screening strength and the charge density modulation; I then present the results on the existence of intra-gap bound state around a single Kondo hole in the heavy Fermi liquid regime; Finally, I discuss the impurity resonance states in different topological phases of Kondo insulators.

10:20—10:40 **Break**

- 10:40—11:20 **P. Hofmann:** *Electronic Structure and Electron Dynamics in Two-Dimensional Materials*
Changing the dimensionality of a material results in significant modifications of its electronic properties. This is even the case if the parent material already has a layered structure with little interaction between the layers, as in the case of graphene, bilayer graphene and single-layer transition metal chalcogenides. This talk discusses the possibility to epitaxially grow high-quality two-dimensional materials on single crystal surface, such that they can be used for electronic structure investigations by time- and angle-resolved photoemission spectroscopy. Results of such studies are presented for graphene, bilayer graphene and single-layer MoS₂.
- 11:20—Noon **A. Balatsky:** *Dirac Materials*
Recently discoveries of graphene and topological insulators have brought a new focus to materials, we call Dirac materials, where quasi-particle behavior is described by very same Dirac equation that governs behavior of relativistic particles. Dirac fermionic spectrum leads to very unusual properties, including Klein paradox, chirality of carriers and impurity states. These properties represent universal consequences of the symmetries that protect the Dirac spectrum of these materials. I will explore these similarities and quantum imaging of these materials.
- Noon—13:20 **Break for Lunch** at La Terraza (provided by La Fonda Hotel)

13:20—17:00 **Afternoon Session** in the New Mexico Meeting Room

13:20—14:00 **R. McDonald:** *Topological Surface States in the Quantum Limit*

Topological insulators (TIs) are quantum materials with an insulating bulk and topologically protected metallic surfaces. An outstanding challenge in the field of TIs is to reveal the intrinsic quantum transport properties of the topological surface states in the presence of parallel conductance from the bulk. To this end I will present magnetotransport measurements in pulsed magnetic field approaching 100 T. In exfoliated $\text{Bi}_2\text{Te}_{3-x}\text{S}_x$ the sulfur composition is shown to chemically tune the band filling, making the surface state quantum limit accessible to pulsed magnetic fields. The Berry phase of the resulting Landau spectrum reveals the strong spin-orbit coupling and Dirac nature of the surface state. The ambipolar transport properties of $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ thin film FET devices in pulsed magnetic fields, exhibit a complex and systematic evolution of magnetoresistance (MR) as the Fermi level is tuned across the Dirac point by gate voltage. In particular, an unusual negative MR prevails at the charge neutral point and gradually becomes positive at higher band filling. This intriguing phenomenon is related to the exotic nature of surface states in the extreme quantum limit.

14:00—14:40 **D. Yarotski:** *Pumped Probes and Topological States*

Dirac materials exhibit exotic physical phenomena and promise numerous applications in electronic, energy and information technologies. Here, we discuss an application of powerful ultrafast optical spectroscopic techniques to reveal the dynamic non-equilibrium behavior of several classes of Dirac materials. In graphene, our experiments demonstrate that photogenerated relativistic carriers transiently enhance Drude-like optical conductivity before transferring the energy to optical phonons on a sub-100-fs time scale. The observed nonlinear scaling of conductivity bursts with photoinduced carrier density sets graphene apart from conventional materials, and provides a new insight into the intra- and inter-band charge scattering dynamics in this unique material. Topological insulators represent a new state of Dirac matter where insulating bulk is surrounded by a conducting surface. We apply terahertz spectroscopy at low temperatures to separate the bulk from the surface transient response, and directly probe the non-equilibrium dynamics of free carriers in thin Bi_2Se_3 films. Our results indicate that short-lived bulk carriers co-exist with the long-lived surface carriers which have higher mobility and can be accessed independently below certain film thicknesses. Finally, femtosecond optical pump-probe spectroscopy of topological crystalline insulators $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$, characterized by a Dirac metallic state on their high-symmetry surfaces, unveil the evolution of transient material response across the topological phase transition driven by doping and temperature variation.

14:40—15:00 **Break**

15:00—15:40 **A. Mohite:** *Properties of Chalcogenites*

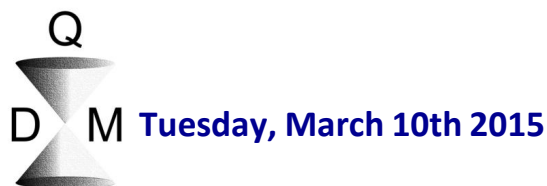
15:40—16:00 **M. Månsson:** *Towards Sodium-based Solid State Energy Storage*

Li-ion batteries are generally considered the main candidate for mobile solid state energy storage applications. However, devices based on lithium's heavier cousin, sodium (Na), have recently received increased attention. One reason is that our Li-reserves are limited and to realize future electric vehicles we might have to reconsider the Li-ion technology. Na has indeed many advantages over Li *e.g.* Na is one of the most abundant elements in nature (earth's crust as well as in normal seawater of our great oceans), which makes it about 5 times cheaper than Li. Further, Na-ion batteries are also much less toxic and easier to recycle. In many ways the Na_xCoO_2 compound is a Na-analog of the most common Li-ion battery electrode material Li_xCoO_2 . Hence, understanding Na-ion diffusion mechanisms in Na_xCoO_2 would seem a logical first step. Here, I will give an introduction to how neutron and muon based techniques are crucial for the understanding of these materials. I will also summarize our recent data from Na_xCoO_2 that reveal how the ion-diffusion process is intrinsically linked to a series of subtle structural transitions along with novel and functional possibilities for tuning battery performance using lattice-strains. Finally, I will show how an understanding of high-temperature ion dynamics can be used to tune low-temperature correlated electron physics in these layered materials.

16:00—16:40 **O. Tjernberg:** *ARPES on Crystalline Topological Insulators*

In this seminar, topological crystalline insulators will be introduced and key differences between topological insulators and topological crystalline insulators highlighted. The key results on topological crystalline insulators that have been achieved so far will be presented including the spin properties, details of the topological phase transition and the spontaneous mass acquisition occurring in connection to crystal symmetry breaking.

17:00—19:30 **Speaker – Participant discussions**



7:30—9:00 **Breakfast** in the Santa Fe Meeting Room (provided by La Fonda Hotel)

9:00—12:00 **Morning session** in the New Mexico Meeting Room

9:00—9:40 **J. Edge:** *Multiband Effects in Interfacial Superconductors*

We investigate the temperature dependence of the upper critical field H_{c2} as a tool to probe the possible presence of multiband superconductivity at the interface between LaAlO_3 and SrTiO_3 (LAO/STO). The behavior of H_{c2} can clearly indicate two-band superconductivity through its nontrivial temperature dependence. For the disorder scattering dominated two-dimensional LAO/STO interface we find a characteristic non-monotonic curvature of the $H_{c2}(T)$. We also analyse the H_{c2} for multiband bulk STO and find similar behavior.

9:40—10:00 **J. Paaske:** *Magnetic Adatoms on Spin-Orbit Coupled Surfaces*

Motivated by experiments on arrays of Fe on a Pb surface, and of transition metal impurities on topological insulator surfaces, this talk will address various aspects of magnetic adatoms on surfaces in which the conduction electrons experience strong spin-orbit coupling. The magnetic ordering in adatom spin chains depends strongly on electron mediated exchange coupling and magnetic anisotropy, both of which turn out to have interesting properties on a spin-orbit coupled substrate.

10:00—10:20 **Break**

- 10:20—11:00 **D. Abergel:** *One Dimensional Excitons*
It has been predicted that excitons comprised of spatially separated ground-state electrons and holes may form a condensate in two-dimensional systems such as double layer graphene. However, this phenomenon has not been experimentally observed in the absence of magnetic field. We analyze the role of charged impurity disorder, and find that it is a crucial limiting factor on the formation of the condensate, implying that device quality is of paramount importance. We then generalize this concept to parallel one-dimensional systems, such as core-shell nanowires.
- 11:00—11:30 **T. Schmitt:** *Resonant Inelastic X-Ray Scattering on One-Dimensional Cuprate and Oxide Heterostructure Materials*
Resonant inelastic X-ray scattering (RIXS) is a powerful bulk-sensitive photon-in/photon-out spectroscopic probe of the electronic structure with atomic and orbital sensitivity. It is an ideal method for studying excitations from the electronic ground state in correlated transition metal oxides, being directly sensitive to charge-, orbital- and spin-degrees of freedom [1]. In this talk we present high-resolution RIXS studies of magnetic and electronic excitations in one-dimensional cuprate and oxide heterostructure materials performed at the ADvanced RESonant Spectroscopies (ADRESS) beamline of the Swiss Light Source [2].
- 11:30—12:00 **E.J. Sie (Gedik Group):** *Breaking Time-reversal Symmetry in WS_2 with Light*
Abstract: Monolayer semiconductors, such as WS_2 , have a pair of valleys that, by time-reversal symmetry, are energetically degenerate. Lifting the valley degeneracy in these materials is of great interest because it would allow for valley specific band engineering and offer additional control in valleytronic applications. Here we show that circularly polarized light, which breaks time-reversal symmetry, can be used to lift the valley degeneracy by means of the optical Stark effect [1]. We demonstrate that this effect is capable of raising the exciton level in monolayer WS_2 by as much as 18 meV in a controllable valley selective manner. The resulting energy shift is extremely large, comparable to the shift that would be obtained using a very high magnetic field (~ 100 Tesla). These results offer a novel way to control valley degree of freedom, and may provide a means to realize new valley-selective Floquet topological state of matter.
- 12:00 —12:40 **A. Taylor:** *Ultrafast Dynamics in Correlated Electron Materials*
Strong correlations between spin, charge, lattice, orbital degrees of freedom play an important role in the emergent properties of correlated electron materials. The unifying theme among all correlated electron materials is the existence of electronic, magnetic and structural spatial inhomogeneities at sub-nanometer-to-micrometer scales and closely related nontrivial picosecond dynamics in response to transient stimuli. The characteristic length and time scales of these inhomogeneities are of extreme interest because they contain information about the underpinning correlations between multiple order parameters. Ultrafast spectroscopies enable the ability to temporally, and recently, spatially, resolve phenomena at the fundamental timescales of atomic and electronic motion. Here, we will review our recent results on ultrafast optical studies of spin, charge, and lattice dynamics, and more importantly, of the dynamics of the coupling between these degrees of freedom in a broad range of correlated electron materials, including heavy fermions, high temperature superconductors, magnetic materials, and multiferroics. We will also describe our tabletop ultrafast time-resolved coherent x-ray capabilities and provide a perspective on their application to correlated electron materials studies.
- 12:40—13:30 **Break for Lunch at La Terraza** (provided by La Fonda Hotel)

- 13:30—17:40 **Afternoon Session** in the New Mexico Meeting Room
Discussions - *Future Initiatives – Collaborative Efforts*
- 13:30—13:45 **L. Kari**- Dean, School of Science: *Research at KTH*
- 13:45—14:00 **A. Bishop** - Principle Associate Lab Director: *Research at Los Alamos*
- 14:00—14:15 **U. Karlsson** – Professor and Materials Platform Head: *KTH Materials Platform*
- 14:15—14:30 **J. Sarrao** - Associate Lab Director: *Theory, Experiment Matter in Extreme Conditions*
- 14:30—14:45 **W. Gudowski**, PI, Head: *Nuclear Reactor Research in KTH*
 Research at KTH covers all important aspects of nuclear technology today and in the future. Three nuclear technology departments in the School of Science together with research groups in Nuclear Chemistry, Nuclear Material Mechanics and Nuclear Safety Philosophy count up to more than 30 senior researchers and well above 30 PhD students. Those scientists are also deeply involved in the Master Program in Nuclear Energy Engineering, one of the best Master Programs in Europe having annually about 30 undergraduate students.
 Material related research is an important part of the nuclear technology development at KTH. The paper will present development of advanced nuclear fuel like nitride, carbide and silicide fuels being tested for heavy metal coolant environment. Another important research focus is Sacrificial Materials of the Ex-Vessel Core Catcher. Experimental research is well supported by computer simulations of materials for nuclear energy technology, in particular: diffusion in nitride fuels, embrittlement and radiation induced segregation in ferritic steels and swelling in bcc and fcc materials.
- 14:45—17:00 **3 Round Tables** – The New Mexico Meeting Room
- Round table 1 Materials In Extreme - *Magnet Lab, MARIE, LUMOS, CINT:***
C. Mielke, A. Taylor, Q. Jia, J. Sarrao, C. Barnes, A. Bishop (LANL); U. Karlsson, M. Månsson,(KTH); J. Fransson (UU)
- Round table 2 Materials for Nuclear Energy - *Nuclear reactor safety and Nuclear Energy Programs:***
M. Caro, O. Anderoglu, N. Mara (LANL); W. Gudowski (KTH)
- Round table 3 Computational Materials Initiative And F- Electron Actinide Materials Database:**
J.Wills, J. Zhu, C. Batista, J. Sarrao, A. Taylor, A. Bishop, D. Clark (LANL); O. Eriksson (UU)
- 17:00—17:40 **Summary** of Round Table discussions
- 17:40—19:30 **Discussions** and wrap-up



Wednesday, March 11th 2015

- 7:30—9:00 **Breakfast** in the Stiha Room (provided by La Fonda Hotel)
- 9:00—12:00 **Morning session** in the Stiha Room (with short coffee break)
- 9:00—12:00 **Round Table wind-up** session (*end time is tentative*)
- 14:30—17:45 **Tour of Los Alamos Facility** – by pre-arrangement with A. Balatsky
- 12:45 **Meet** in front of Hotel Reception for transportation to Los Alamos
- 12:55 – 14:00 Travel to Los Alamos National Laboratory
- 14:00 – 14:30 Los Alamos Badge office to get badges
- 14:30 – 15:30 CINT tour, Jia Quanxi
- 15:30 – 16:00 CNLS tour, Robert Ecke and Aric Hagberg
- 16:15 – 17:45 NHMFL tour, Charles Mielke
- 18:00 Assemble for return transportation to Santa Fe

